

Title:

NEW MCNPX DEVELOPMENTS

Author(s):

John S. Hendricks, Gregg W. McKinney,
Laurie S. Waters, H. Grady Hughes III,
Edward C. Snow

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John S. Hendricks
Los Alamos National Laboratory
Nuclear Systems Design and Analysis Group
P.O. Box 1663, MS K575
Los Alamos, NM 87545
505-667-6997
jxh@lanl.gov

Laurie S. Waters
Los Alamos National Laboratory
Nuclear Systems Design and Analysis Group
P.O. Box 1663, MS K575
Los Alamos, NM 87545
505-665-4127
lsw@lanl.gov

Gregg W. McKinney
Los Alamos National Laboratory
Nuclear Systems Design and Analysis Group
P.O. Box 1663, MS K575
Los Alamos, NM 87545
505-665-8367
gwm@lanl.gov

H. Grady Hughes, III
Los Alamos National Laboratory
Transport Methods Group
P.O. Box 1663, MS D409
Los Alamos, NM 87545
505-667-5957
hgh@lanl.gov

Edward C. Snow
TechSource, Inc.
1418 Luisa
Santa Fe, NM 87594-1057
865-574-9675
esnow@hillsboro.net

SUMMARY

The Los Alamos National Laboratory Monte Carlo N-Particle extended (MCNPX)¹ radiation transport code has been upgraded significantly to Version MCNPX2.4.0.* It is now based on the latest MCNP4C3² and MCNPX2.3.0 releases to the Radiation Safety Information Computational Center (RSICC). In addition to all of the advances from earlier versions of MCNP and MCNPX, important new capabilities have been developed.

I. INTRODUCTION

The Monte Carlo method³ was developed at Los Alamos National Laboratory during the Manhattan Project in the early 1940s. MCNP and MCNPX are heirs to those early efforts. Over 400 person-years have been invested in the research, development, programming, documentation, and databases for these codes.

MCNP is a general-purpose neutron (0-MeV to 20-MeV), photon (1-keV to 1-GeV), and electron (1-keV to 1-GeV) transport code for calculating

the time-dependent, continuous-energy transport of these particles in three-dimensional geometries. MCNP is perhaps the most widely used and well-known physics simulation code in the world today.

MCNPX extends MCNP to track nearly all particles at all energies. MCNPX combined MCNP and the LAHET Code System (LCS).⁴ LCS is based on the Oak Ridge High Energy Transport Code.⁵ LCS uses models for particles in physics regimes where there are no tabulated data, including the Bertini⁶ and ISABEL⁷ models. MCNPX has additional models to LCS, such as the CEM model.⁸ MCNPX2.3.0⁹⁻¹¹ was released to RSICC in December 2001 and is based on MCNP4B.¹² The principal features of MCNPX2.3.0 are

- ☐ Physics for 34 particle types;
- ☐ High-energy physics above the giga-electron-volt range;
- ☐ Neutron, proton, and photonuclear 150-MeV libraries;
- ☐ Photonuclear physics;
- ☐ Mesh tallies;

*MCNPX, MCNP, LAHET, and LCS are trademarks of the Regents of the University of California, Los Alamos National Laboratory.

- Radiography tallies;
- Secondary particle production biasing;
- VAVILOV energy straggling for charged particles; and
- Automatic configuration for compilation.

The focus of this work is MCNPX2.4.0, which is due for imminent release. MCNPX2.4.0 merges MCNPX2.3.0 with MCNP4C3 and adds important new features.

II. NEW MCNP FEATURES FOR MCNPX USERS

MCNPX2.3.0 is based on MCNP4B. The new MCNPX2.4.0 is based on MCNP4C3 and gives MCNPX users the following additional MCNP4C3 capabilities:

- Easier geometry specification with macrobodies;^{13,14}
Though MCNPX retains its surface-sense geometry, the new macrobodies make geometry specification much easier—such as the combinatorial geometry of the Integrated Tiger Series.¹⁵
- Improved variance reduction with the superimposed mesh weight window generator;^{16–19}
No longer do geometries have to be subdivided for importances. A weight window mesh now can be superimposed over geometries and the appropriate variance reduction parameters automatically generated.
- Superimposed mesh plotting;²⁰
The weight window mesh may now be plotted.
- Interactive geometry plotting;²¹
Geometry plots may still be done in command mode, but a new point-and-click capability makes geometry plotting much easier and more interactive.
- Delayed neutrons;²²
Delayed fission neutrons are now modeled with optional biasing.
- Unresolved resonance range probability tables;²³

Neutron data above the resolved resonance range are now much more correctly modeled.

- Perturbations for material-dependent tallies;²⁴
The second-order differential operator perturbation capability has been upgraded significantly.
- ENDF/B-VI extensions;²⁵
New data formats of the ENDF/B-VI data libraries are now accommodated in MCNP4C. The ENDF/B-VI extensions are also in MCNPX2.3.0 but were not in the previous MCNPX2.1.5 release to RSICC.
- PC enhancements;
MCNPX now compiles, runs, and plots with Microsoft Windows[TM].
- Electron physics enhancements (upgrade to ITS3.0);¹⁵
The electron physics in MCNP and MCNPX is based on the Integrated Tiger Series of codes (ITS)¹⁵ from Sandia National Laboratories (SNL). MCNP4C adds to MCNPX2.4.0 the upgrade to ITS3.0.
- Parallelization enhancements; MCNP and low-energy MCNPX neutron/photon/electron problems now run in parallel with either distributed- or shared-memory multiprocessing with PVM and OpenMP.
- Weight window enhancements. Weight windows may now be time-dependent or scaled by a factor. Performance has improved in unspecified weight window regions for better compatibility with weight cutoffs.

Many of these capabilities have required more than just putting MCNP and MCNPX together: they were integrated. MCNPX features such as improved particle summary and balance table coding had to be extended to the MCNP parts of the code. Extensions beyond MCNP4B, such as ENDF/B-VI extensions and photonuclear reactions,²⁶ had been put into MCNP4C and MCNPX in very different ways, which had to be reconciled. New features, such as macrobodies, having nothing to do with high-energy physics models, nonetheless required changes to high-energy physics modules because of variable name conflicts or changes in subroutine calls. New MCNP features, such as superimposed mesh weight windows, had to be made compatible with the high-energy transport routines.

III. NEW FEATURES FOR MCNP USERS

MCNPX2.4.0 offers MCNP users not only physics for 34 particle types and high-energy physics above the giga-electron-volt range, but also many standard MCNPX features of use for low-energy neutrons, photons, and electrons.

- Mesh tallies.
The MCNPX mesh tallies make it possible to plot particle tracks, source locations, and energy deposition on a grid superimposed over any arbitrary portion of the problem geometry.
- Radiography tallies.
Next-event estimators have been extended to radiography tallies, which model either pinhole radiography or fluoroscopic images. Examples would be a patient emitting radiation from a radioactive dose such as in positron-emission therapy, or a high-energy x-ray of luggage at an airport.
- Automatic configuration for compilation.
The MCNPX installation package automatically determines the available compilers, library locations, and other aspects of a system to configure and then compile MCNPX appropriately and easily.

IV. NEW MCNPX2.4.0 FEATURES

Additionally, MCNPX2.4.0 has many new capabilities not found in either MCNP4C or MCNPX2.3.0.

- FORTRAN 90 modularity and dynamic memory allocation.
The only available Microsoft Windows compilers are F90 and F95, and F77 compilers (for which MCNP4C3 and MCNPX2.3.0 are designed) are becoming increasingly unreliable and obsolete. There is a time penalty for F90, but improvements have been made in code modularity, standardization of functions such as timing across platforms, and compiler reliability.

Note that MCNPX2.4.0 can be modified by patches, and as much of the MCNP4C coding as possible has been preserved so that MCNP4C patches can be applied directly to MCNPX2.4.0.

- Repeated structures source path improvement.

Sources in repeated structures and lattices may now be specified with the same notation as tallies, and the paths are correctly printed in the output.

- Smaller enhancements.
MCNPX also contains some error corrections to MCNPX2.3.0 and MCNP4C3; improvements in output; significantly faster plotting of long repeated structures/lattice problems; speedup of MCNPX n,p,e problems by not looping over unused particles; and more.

Under development—may not be in initial MCNPX2.4.0 release:

- Pulse height tallies with variance reduction.
- Distributed-memory parallel processing for high-energy applications.
- French Cugnon Intranuclear Cascade (INC) Model.
- Built-in link to VISED setup code.²⁷
- Mix and Match Capability.
In the neutron (and other particle) energy range above the top energy of some data libraries but below the top energy of other libraries, MCNPX currently cannot mix both model and tabular data. Either the higher-energy data are ignored and models are used for all nuclides, or the data are used where they exist and are extrapolated from the top of the energy table for nuclides where the data do not exist. A means of mixing and matching both tabular data and model data is being developed for these cases.
- Built-in dose functions. Many standard dose functions are available, thus eliminating the need to input DE/DF cards manually and laboriously.
- Special features for space applications.²⁸

These developments in MCNPX significantly upgrade its usefulness for the radiation protection and shielding community.

V. SUMMARY

For MCNPX users, MCNPX2.4.0 provides the significant upgrade in features from MCNP4B to MCNP4C3 and from MCNPX2.1.5 to MCNPX2.3.0. For MCNP users, MCNPX2.4.0 provides not only all-particle high-energy transport, but also mesh tallies,

radiography tallies, and automatic configuration installation. For both MCNPX and MCNP users, MCNPX provides F90 Fortran capabilities and many new features that make it an effective tool for radiation protection and shielding applications.

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